Advanced Research Center for Beam Science
- Electron Microscopy and Crystal Chemistry -

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Visitors

Prof YUAN, J	Tsinghua University, China, 12 June 2004
Dr MAGONOV, S	Digital Instruments/Veeco Metrology, USA, 14 June 2004
Prof MILES, M, J	H.H.Wills Physics Laboratory, University of Bristol, UK, 2 July 2004
Prof CHOU, L,-J	National Tsing Hua University, Taiwan, 12 August 2004
Prof LAI, C,-H	National Tsing Hua University, Taiwan, 12 August 2004
Prof CHEN, H,.-Z	Zhejiang University, China, 15 November 2004

Scope of Research

Crystallographic and electronic structures of materials and their transformations are studied through direct imaging of atoms or molecules by high-resolution spectromicroscopy which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high resolution imaging. It aims to explore new methods for imaging and also obtaining chemical information in thin films, nano-clusters, interfaces, and even in solutions. By combining this with scanning probe microscopy, the following subjects are urging: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, fabrication of low-dimensional functional assemblies.

Research Activities (Year 2004)

Presentations

Cryo-TEM Observation of the Formation Process of Gold Nano-rod in an Aqueous Solution of Surfactant, Ogawa T, Kurata H, Isoda S, International Symposium on the Creation of Novel Nanomaterials, 20 January.

Core Hole Effects on the Oxygen K-ELNES of Transition Metal Oxides, Kurata H, Tsujimoto M, Nemoto T, Isoda S, 8th APEM, 7 June.

Nano-scale Direction Control of 2-dimensional Organic Crystals at Liquid/solid Interface, Nemoto T, Takajo D, Kurata H, Isoda S, 8th APEM, 10 June.

Thin Film Structures and Optical Properties of the Bis(1,2-benzoquinonedioximato) Platinum(II), Yoshida K, Yaji T, Isoda S, EM-NANO 2004, 8 June.

Transport Properties of Single-grain Organic Field-effect Transistor, Minari T, Nemoto T, Isoda S, The International Symposium on Super-Functionality Organic Devices, 26 - 28 October.

Topics

Structures of Adsorbed Initial Layers of Stearic Acid at the Liquid/Solid Interface

The structures of stearic acid adsorbed initially on highly oriented pyrolytic graphite (HOPG) were examined at liquid/solid interfaces by scanning tunneling microscopy (STM). Depending on the concentrations of stearic acid in n-octylbenzene solutions, two structures were observed. For a saturated solution of stearic acid, the observed layer on HOPG was composed of large and stable domains under STM scanning, corresponding with the already reported structure (β-form). For low concentrations, molecular layers were also formed, but at the lowest concentration of 1.7 mM, the molecular layer became porous where an underlying layer with another structure (α-form) was observed. It was concluded that the α-form is the initially adsorbed layer and the second layer is formed as the β-form.

Takajo D *et al., JJAP,* **43**(7B), 4667 (2004).

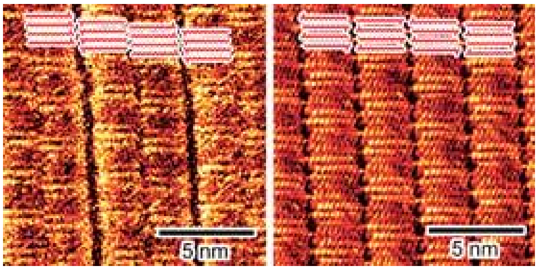

Figure 1. STM images of the α- and β-form stearic acid on HOPG.

DV-Xα Calculation of Electron Energy-Loss Near-Edge Structures of F_4TCNQ

The first principle molecular orbital (MO) calculations, focusing on the carbon K-edge fine structures, were performed for 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-quinodimethane (F_4TCNQ) and 7,7,8,8-tetracyanoquinodimethane (TCNQ). Electron energy-loss spectra (EELS) of F_4TCNQ were measured and analyzed through the calculation. In the discrete variational-Xα(DV-Xα) method, site-excited transition state configurations were assumed to take account of core-hole effects and, consequently, were examined in three parts: (1) partial density of states (PDOS) of unoccupied 2p orbitals; (2) inner 1s orbitals (energy-recalibrated PDOS); and (3) photo-absorption cross-section (PACS) considering the transition matrix. In F_4TCNQ, the inner 1s energy level of the quinoid-ring carbon combined to fluorine shifts deeper in energy, resulting in a high-energy shift of the π^* peaks in the calculation. The calculation also showed the fluorination effect on the quinoid-ring carbons appearing in the higher σ^* energy region. In the low energy region, the calculations accurately reproduced the core-excited spectra in both F_4TCNQ and TCNQ and succeeded in assigning each component appearing in the spectra.

Koshino M *et al., J. Electron Spectroscopy & Related Phenomena,* **135**(2-3), 191, (2004).

Figure 2. Cryogenic electron spectro-microscope: STEM/TEM, Field emission gun, Liquid He cryo-holder, Ω-imaging filter, EELS, 2k×2k CCD detector.

Nanodiffraction and Characterization of Titanate Nanotube Prepared by Hydrothermal Method, Kubota Y, Kurata H, Isoda S, Korea-Japan Joint Forum 2004, 3 - 6 November.

First Principles Calculations of Electron Energy-Loss Near-Edge Structure of Transition Metal Compounds, Kurata H, Tsujimoto M, Nemoto T, Isoda S, IUMRS International Conference in Asia, 15 - 17 November.

Grants

Isoda S, Nanotechnology Support Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2004 - 31 March 2005.

Kurata H, Local State Analysis of Organic Materials by Spatially and Angular Resolved EELS, Grant-in-Aid for Scientific Research (B), 1 April 2003 - 31 March 2006.

Ogawa T, Observation of the Production Process of Metal Nano-rod by Colloidal Method Using Cryo-TEM, Grant-in-Aid for Scientific Research, Promotive Research, 1 April 2003 - 31 March 2005.

Kurata H, Development of an EELS/XES Electron Microscope for Electronic Structure Analysis, Leading Project, The Ministry of Education, Science, Culture and Sports, Japan, 1 April 2004 - 31 March 2006.